Automated Probabilistic Finite Element Model Calibration Tool Based on Uncertainty Quantification and Machine Learning

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Introduction

Background:

- Metallic additive manufacturing (AM) → Laser Powder Bed Fusion (LPBF)
- Laser produced melt pools (~µm) to build parts (~ cm) with millions of scan passes
    - Local variation of defects and microstructure [1, 2] = variation and inconsistencies in part properties
        - Each part printed with a unique set of material properties → qualification and certification (Q&C)

NASA Transformational Tools and Technologies Project (TTT):

- Predict properties and quantify variability to ease hurdles to Q&C [3]
    - High fidelity simulations are very time costly (~100k CPU hours) and still require calibration [4]
        - High-temperature material properties
- Probabilistically calibrate and validate reduced fidelity thermal finite element (FE) model (COMSOL®)

Extract measured data (10 scans) → Calibrate FE Model at each scan → Interpolate between scans

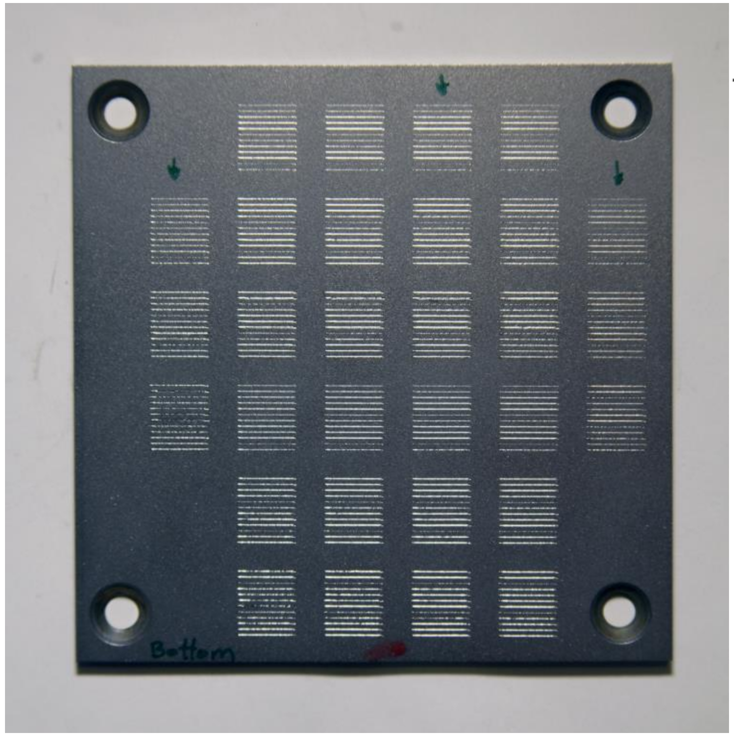
[1] Mahadevan, Sankaran, Paromita Nath, and Zhen Hu. "Uncertainty Quantification for Additive Manufacturing Process Improvement: Recent Advances." ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering 8.1 (2022): 010801.
[2] Herriott, Carl, et al. "A multi-scale, multi-physics modeling framework to predict spatial variation of properties in additive-manufactured metals." Modelling and Simulation in Materials Science and Engineering 27.2 (2019): 025009.
[3] Blakey-Milner, Byron, et al. "Metal additive manufacturing in aerospace: A review." Materials & Design 209 (2021): 110008.
[4] Khairallah, S., Anderson, A., Rubenchik, A., et. al., 2016, "Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones," Acta Materialia, Vol. 108, p. 36-45.

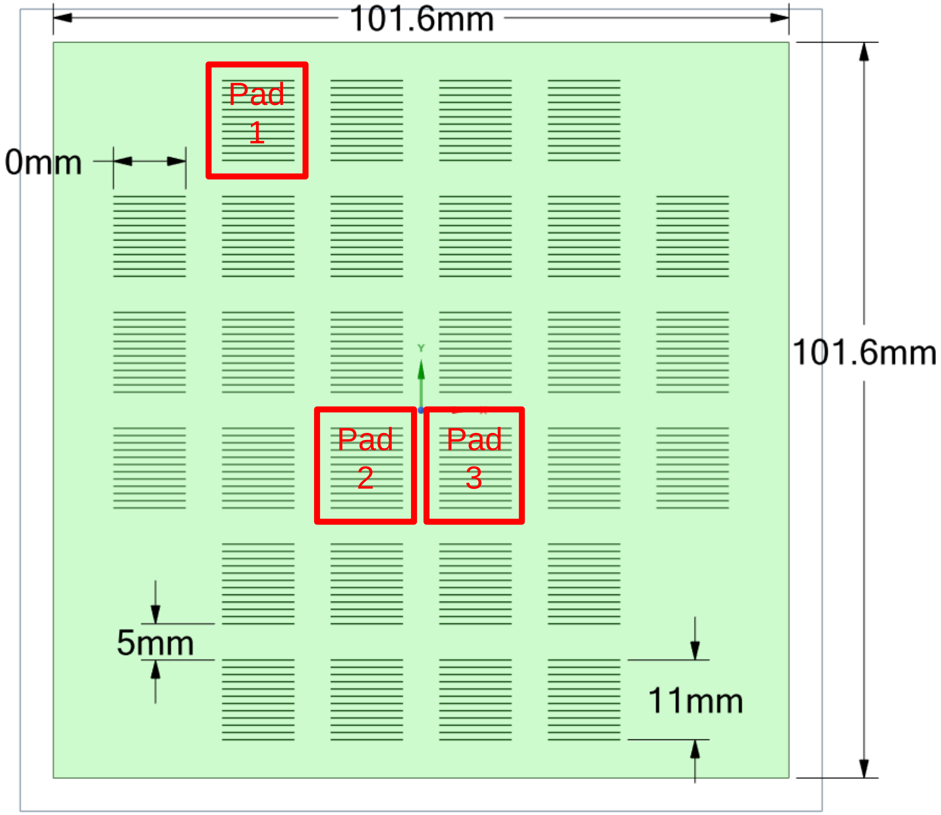
Materials and Test Matrix

Single scan passes on bare Ti-6Al-4V plate:

- EOS M290 LPBF machine at University of Pittsburgh
- Pads each contain scans 1 – 10 (each scan repeats 3 times)
- Process parameters (PPs): laser power and velocity
- 10 scans: 30 serial cross sections → 300 total images

Plate Top Surface





Test Matrix

Scan Number	Power (W)	Velocity (mm/s)
1	225	1250
2	225	1500
3	170	750
4	170	1000
5	170	1250
6	170	1500
7	150	750
8	150	1000
9	150	1250
10	150	1500

EOS M290 default setting. Used to validate interpolator.

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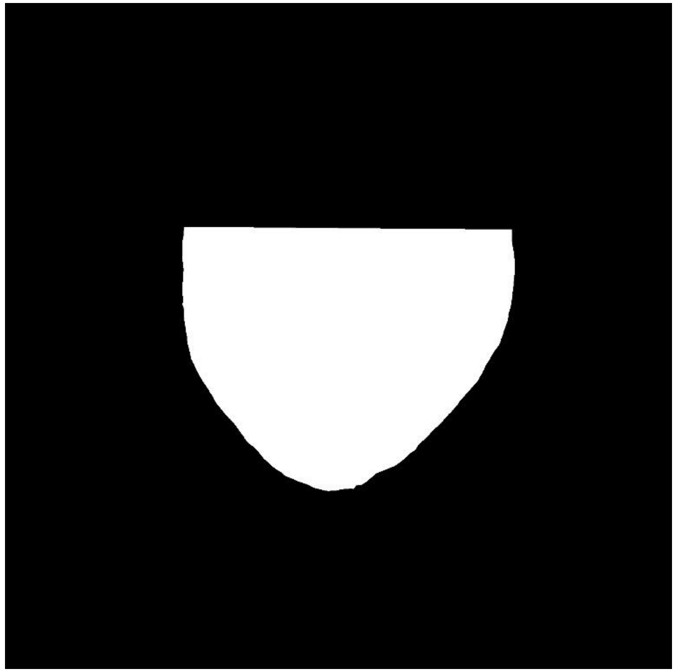
Melt Pool Contour Identification Approach

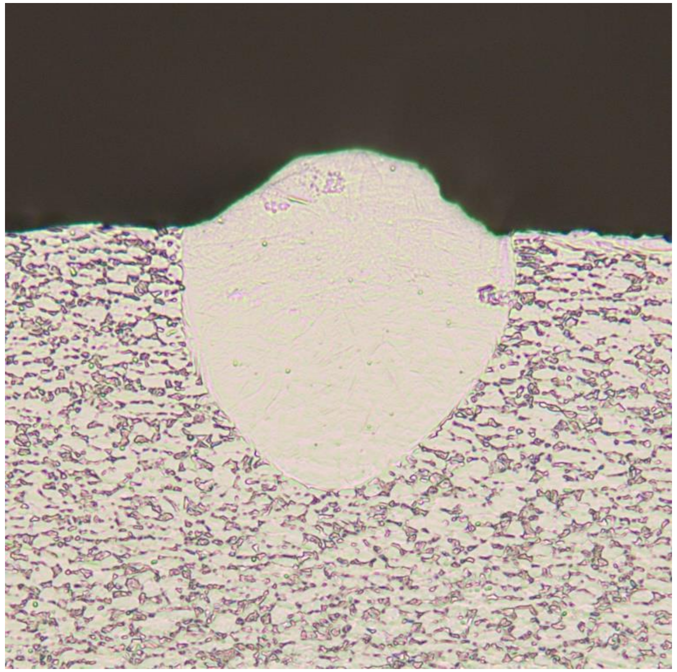
Extract measured data (10 scans) → Calibrate FE Model at each scan → Interpolate between scans

- Required to process large number of images (300 current; thousands in future)
- U-Net architecture (Convolutional Neural Network (CNN))
  - Implemented in Python (TensorFlow) using EfficientNetB3 pretrained image classification model
- Semantic segmentation of an input image into two parts: melt pool and other
- Extrema to identify melt pool dimensions (MPDs): width and depth

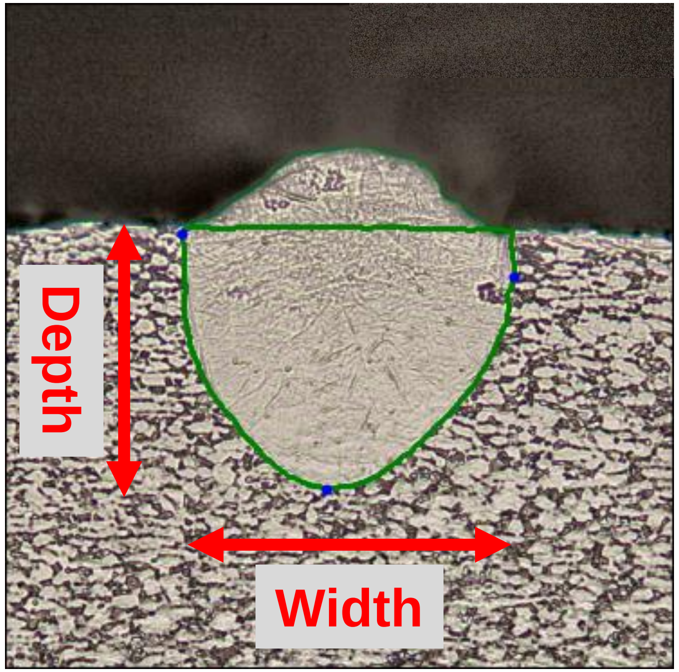
Training Mask



Input Image



CNN Predicted Contour



Melt Pool Contour Identification Results

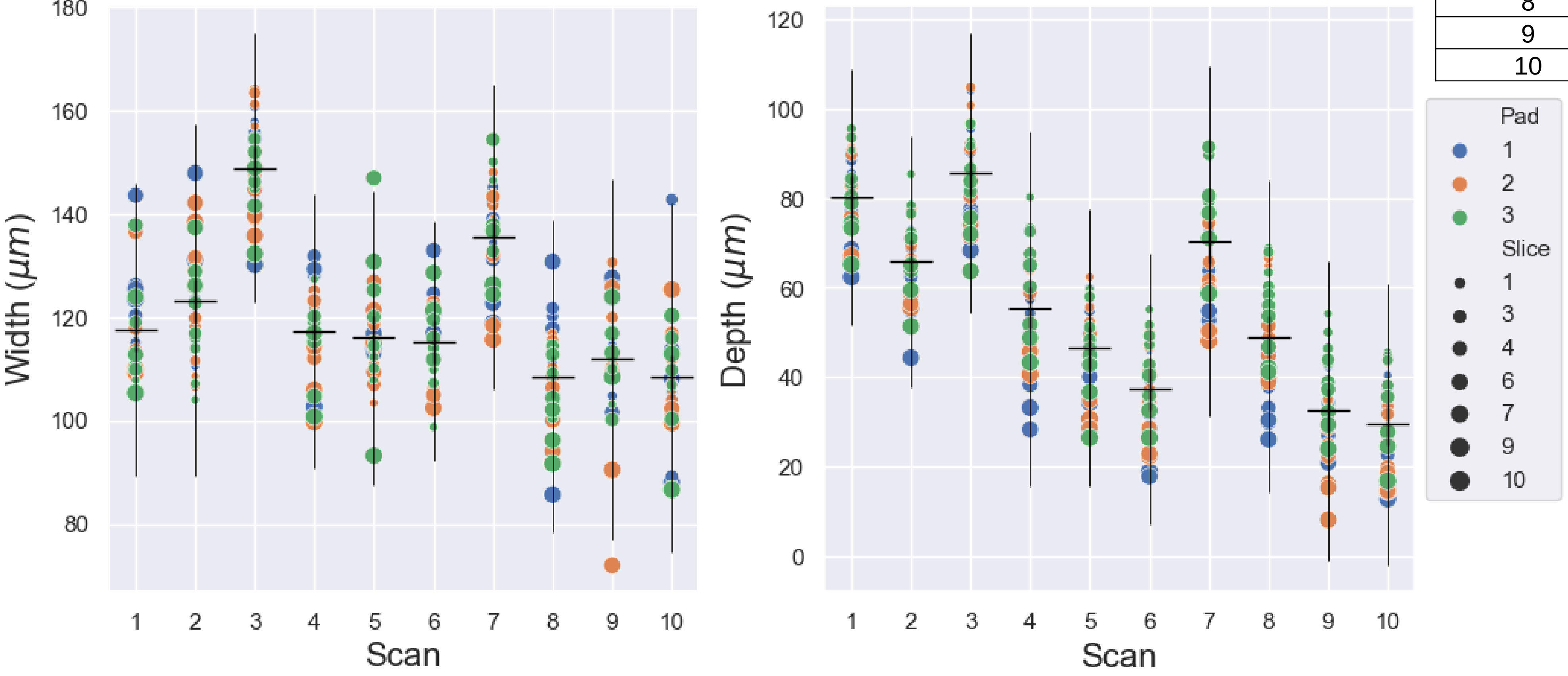
CNN prediction results:

- CNN test set (9 images): average accuracy 95.2% (intersection over union)

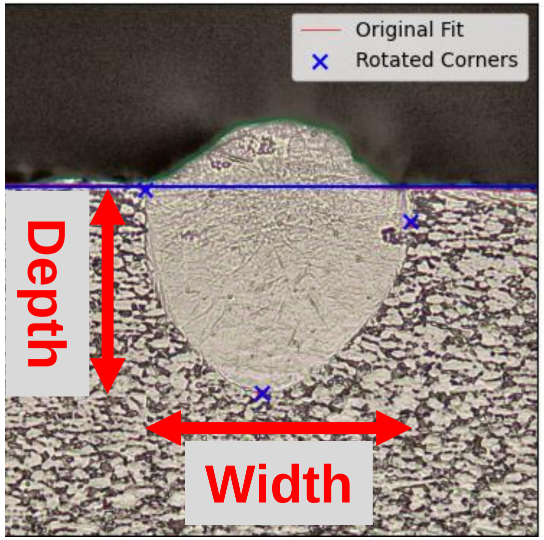
Scan Number	Power (W)	Velocity (mm/s)
1	225	1250
2	225	1500
3	170	750
4	170	1000
5	170	1250
6	170	1500
7	150	750
8	150	1000
9	150	1250
10	150	1500

Melt Pool Width and Depth for all 300 Images

Error bars show +/- 3x Standard Deviation and Mean



Contour Reduction



Probabilistic Calibration Approach

Extract measured data (10 scans) → **Calibrate FE Model at each scan** → Interpolate between scans

Probabilistic calibration of FE model to experimental observations:

- Predict MPDs by tuning FE model heat source parameters at each PP setpoint

Active learning loop

Initialize surrogate

Attempt 6 random points predicted by FE model selected by Latin Hypercube Sampling

Iterative loop efficiently develops surrogate of FE model targeting observed data using Bayesian inference

Final posterior validation

FE Model: Calibrate Volumetric Heat Source

Reduced order FE transient thermal model physics:

- Volume:
  - Heat diffusion
  - Liquid – solid phase change
  - Volumetric laser heat source (Gaussian, based on Goldak [5])
- Surface:
  - Radiation and convection heat loss
  - Liquid – gas evaporation heat loss
- Ignores expensive and uncertain melt pool physics

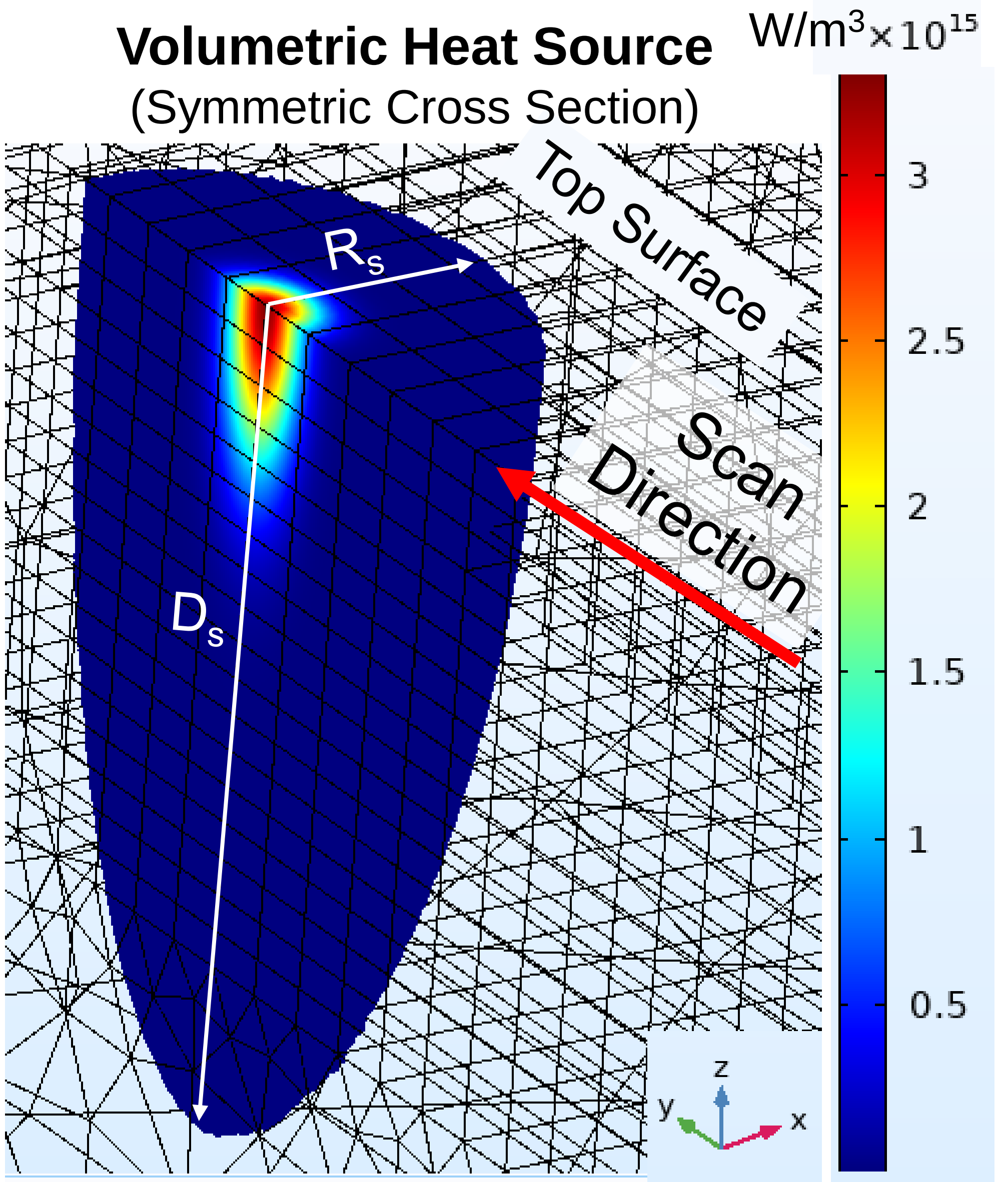
Volumetric heat source calibration variables:

- $\mathbf{R_s}$: heat source radius
- $\mathbf{D_s}$: heat source depth
- $\mathbf{a_{eff}}$: effective laser power absorptivity

Predicted output variables (MPDs):

- Width
- Depth

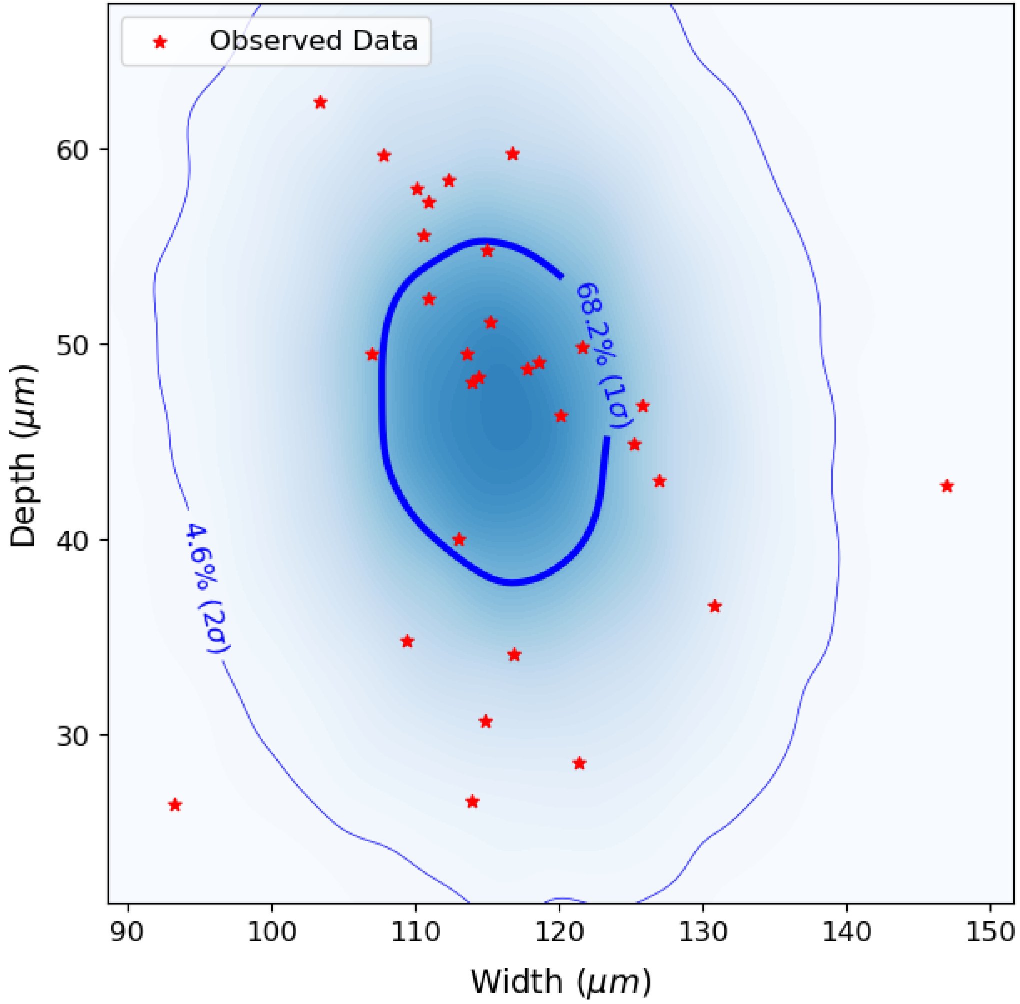
Volumetric Heat Source
(Symmetric Cross Section)



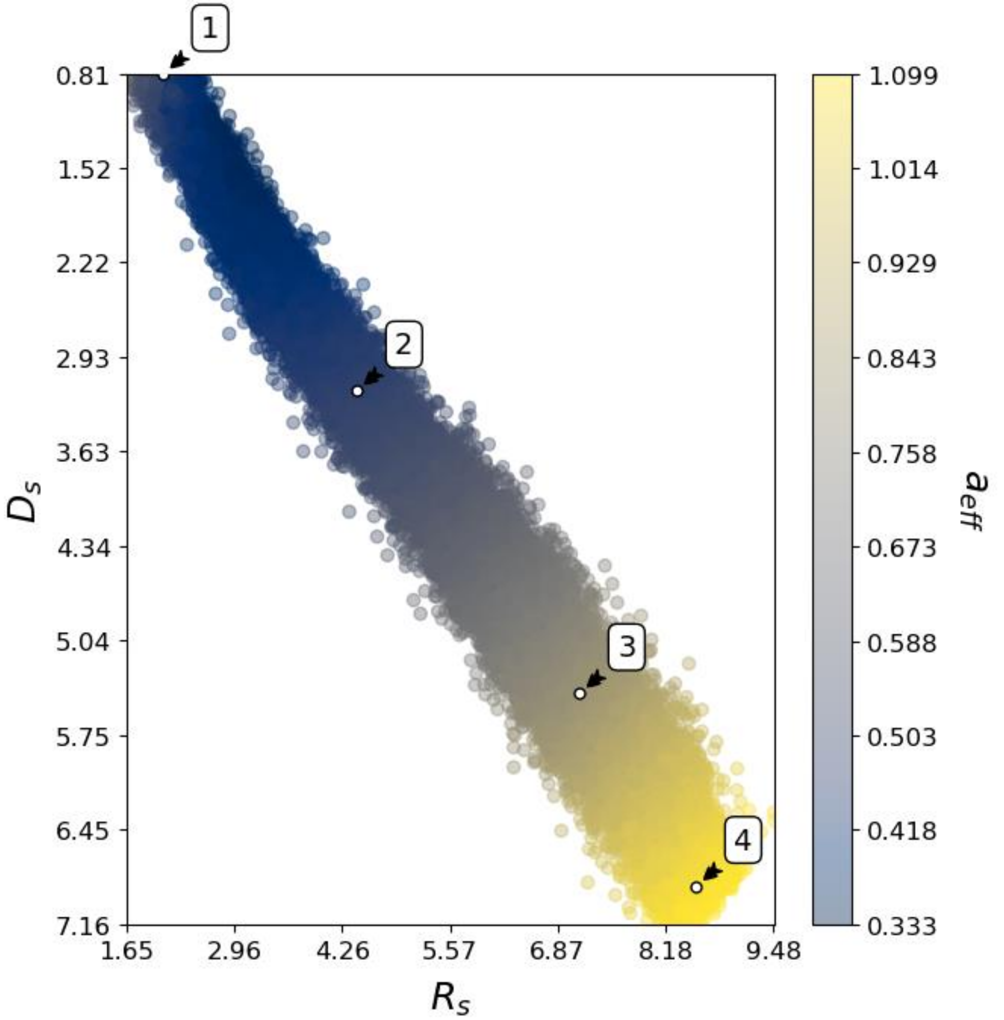
[5] Goldak, J., Chakravarti, A., Bibby, M., 1984, "A New Finite Element Model for Welding Heat Sources," Metallurgical Transactions B, Vol. 15B, p. 299-305.

FE Model Calibration Results (Scan 5)

Surrogate predicted melt pool dimensions for posterior

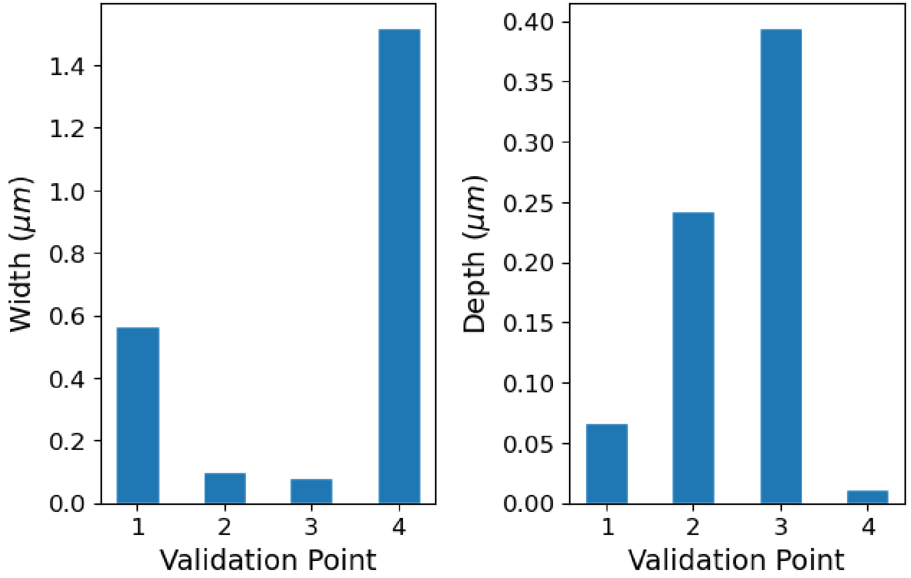


Posterior: distribution of calibrated heat source parameters and 4 selected validation points



Validation of FE Model Calibration Results (Scan 5)

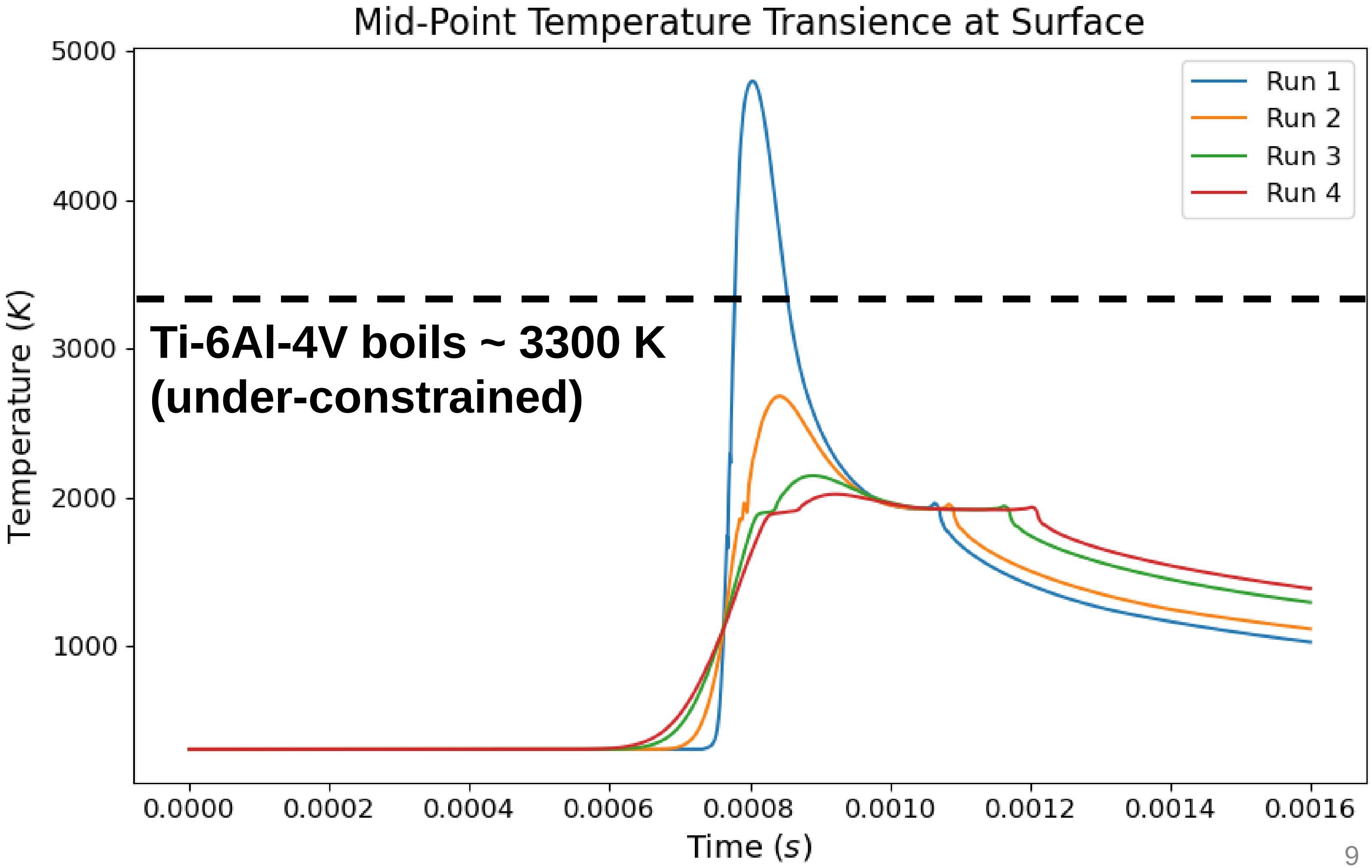
Surrogate validation: Absolute error at 4 validation points



Calibration approach is under-constrained:

- Subset of scan 5 posterior will be used to fit interpolator targeting 3300 K temperature maximum

Temperature history at 4 selected validation points



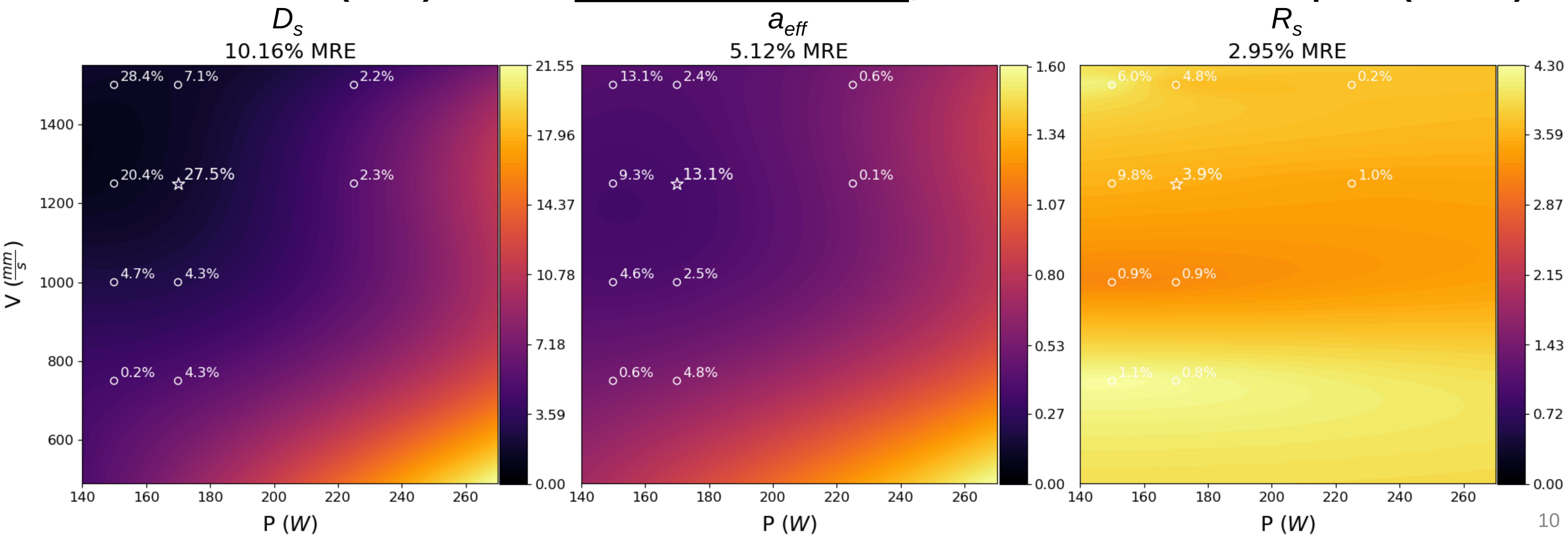
Interpolator: Optimize Fit of Single Points

Extract measured data (10 scans) → Calibrate FE Model at each scan → <u>Interpolate between scans</u>

Gaussian Process Regression optimized using custom grid search:

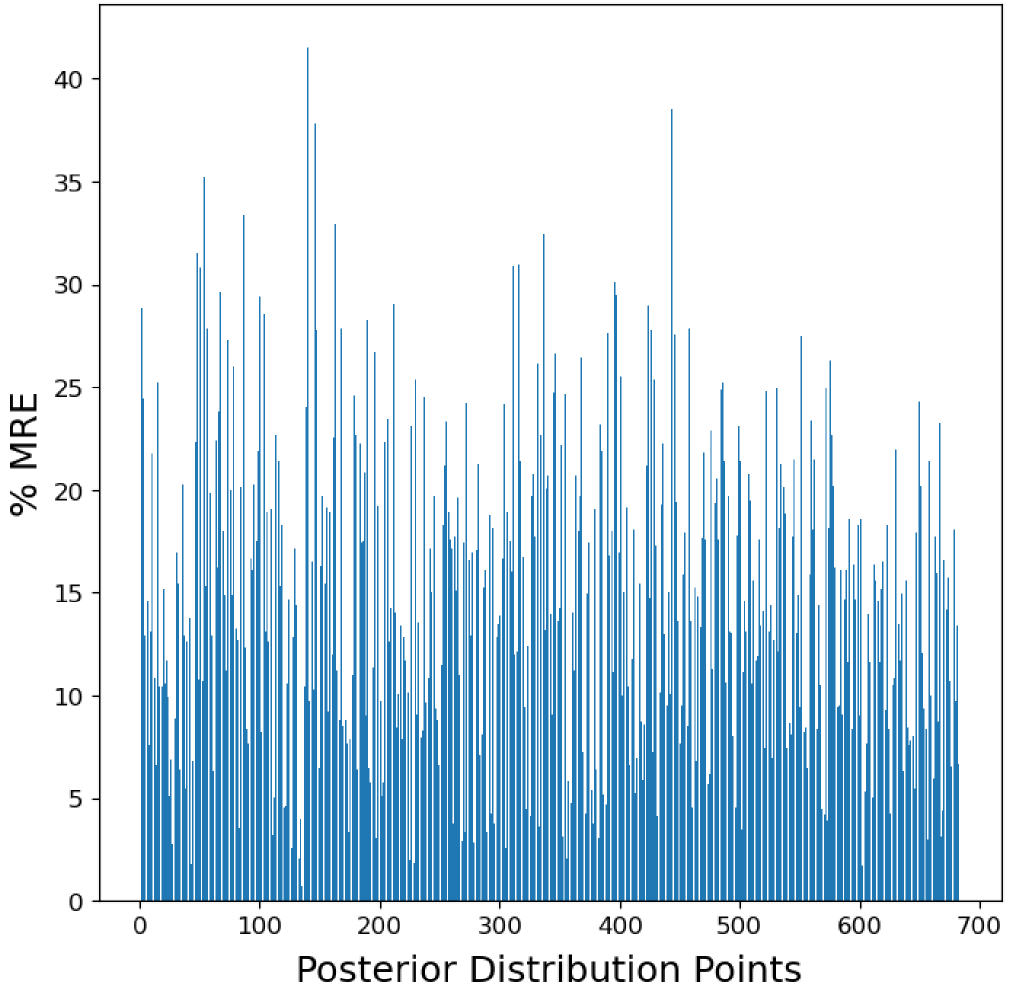
- Separate estimators optimized for each variable (D_s, a_{eff}, R_s) at median posterior point
- “Leave one out” k-folds cross validation for 9 of 10 points; scan 5 reserved (validation point)

Mean Relative Error (MRE) for fit of <u>most probable points</u>; star indicates validation point (scan 5)

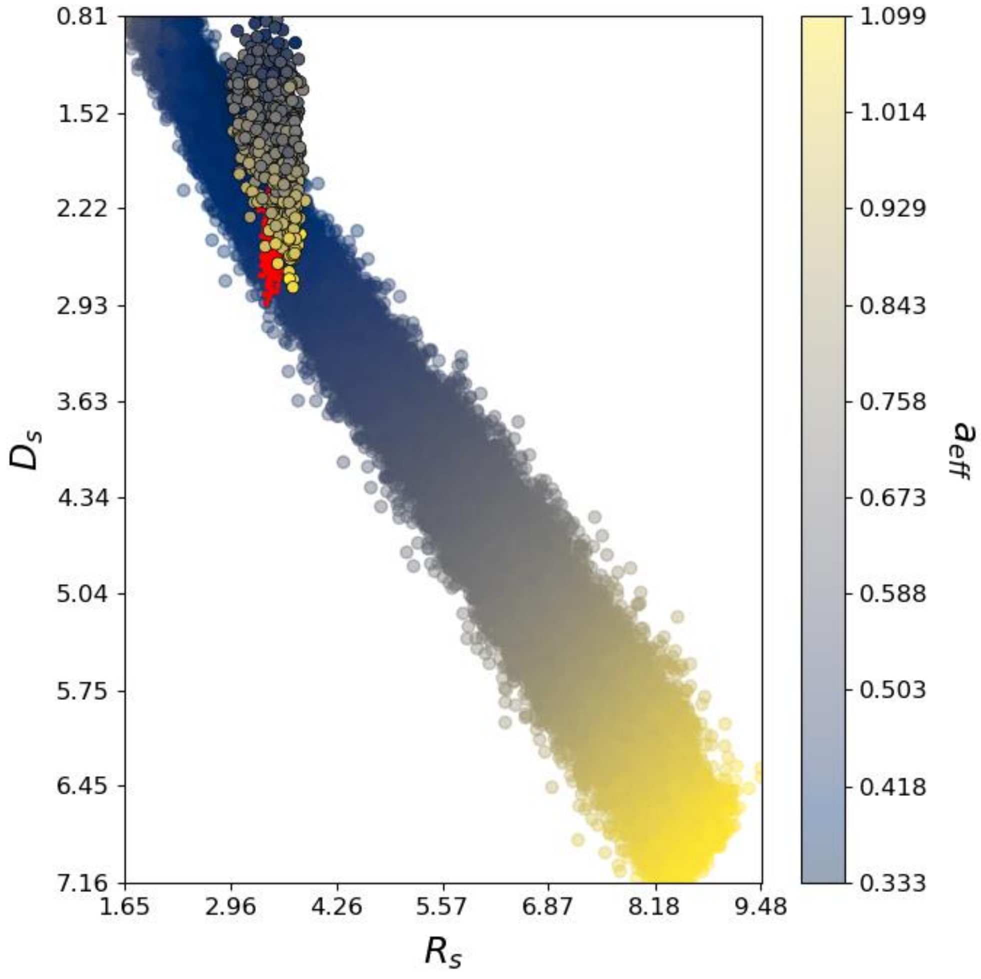


Interpolator Validation: Ensemble of Fits Estimate Distribution

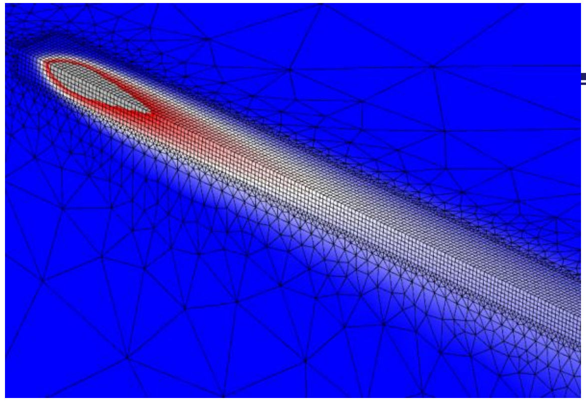
Scan 5 ensemble:
Average MRE over all 3 variables
(global MRE 14.43%)



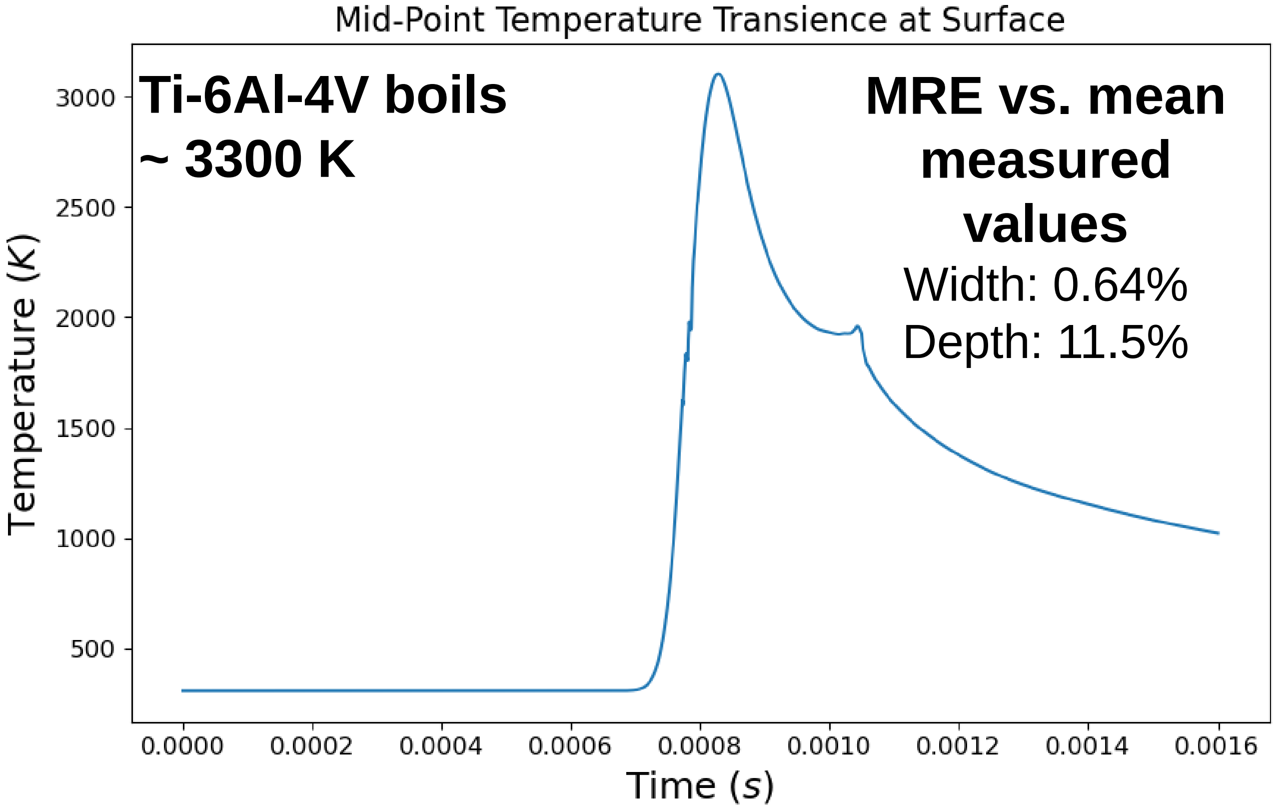
Scan 5 posterior with overlays:
Subset used for fitting (red)
Ensemble predicted subset (black edge)



FE Model Predictions at Interpolated Validation Point



Single validation: most probable point



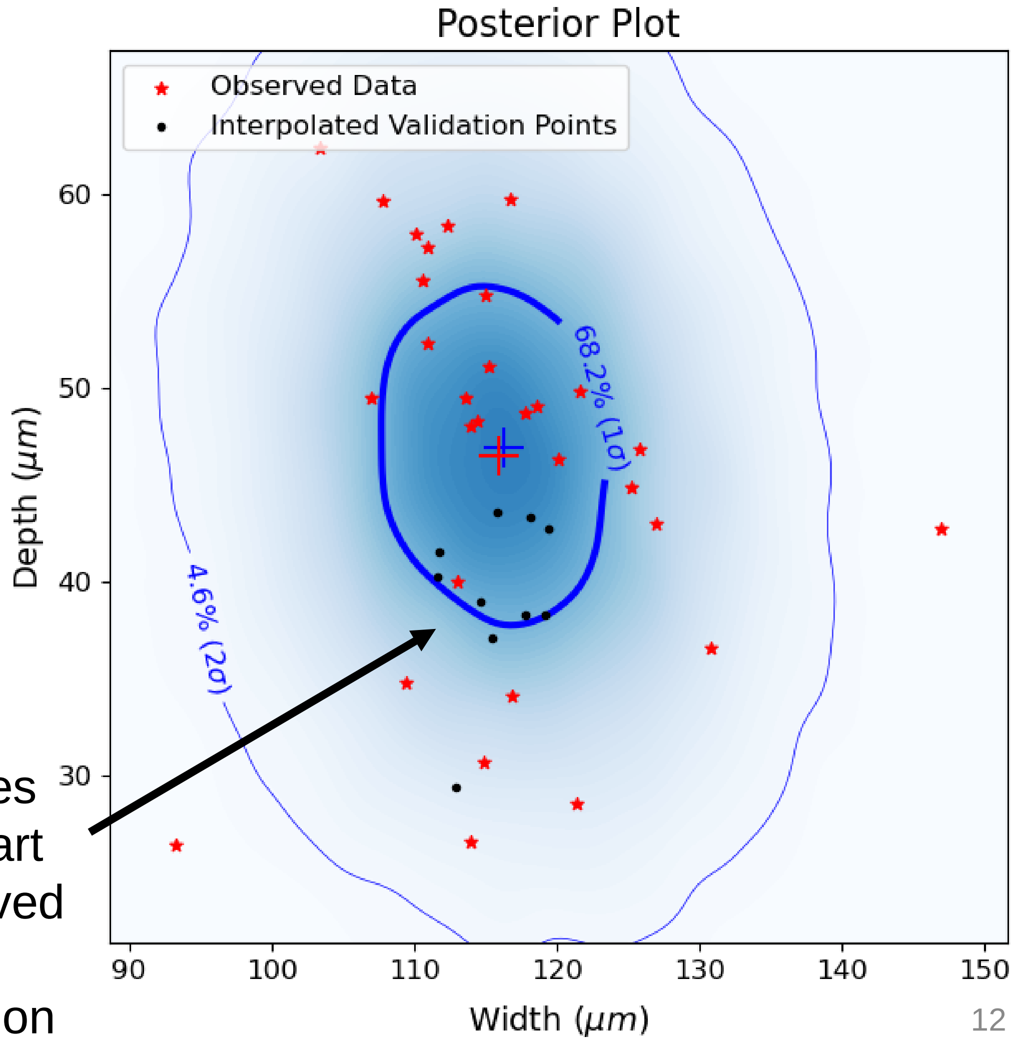
Ti-6Al-4V boils ~ 3300 K

MRE vs. mean measured values

Width: 0.64%

Depth: 11.5%

Probabilistic validation: 10 points over widest range



Captures small part of observed data distribution

Concluding Remarks and Future Work

Summary

- 10 single scan tracks on bare Ti-6Al-4V plate cross sectioned to produce 300 images
- Melt pool width & depth extracted from images using CNN approach (95.2% accuracy on test set)
- Probabilistic calibration of thermal model to width & depth measurements (validation < 1.4 μm for scan 5)
- Ensemble of fits interpolator validated with scan 5
  - Most probable point vs. mean of observed values < 11.5% MRE
  - 10 points sample from posterior predict within 2σ observed values but do not capture full distribution

Future Work:

- Improve interpolator to better describe posterior distribution
  - Fits sensitive to hyper-parameter settings and posterior sub-set used for training and testing
- Further constrain calibration approach:
  - Maximum surface temperature from FE model as a calibration target
  - Target melt pool contour instead of width and depth

Acknowledgements

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CNN approach development

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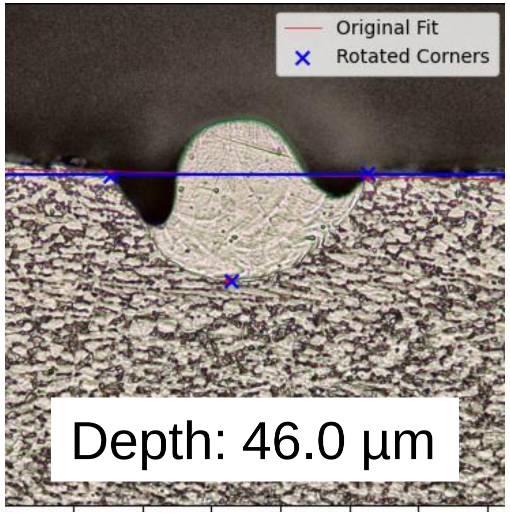
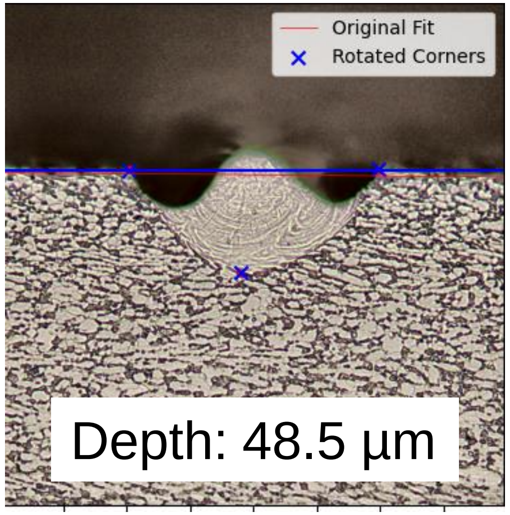
- Hanshen Yu (Worcester Polytechnic Institute)
- Andy Ramlatchan (NASA Langley Research Center)

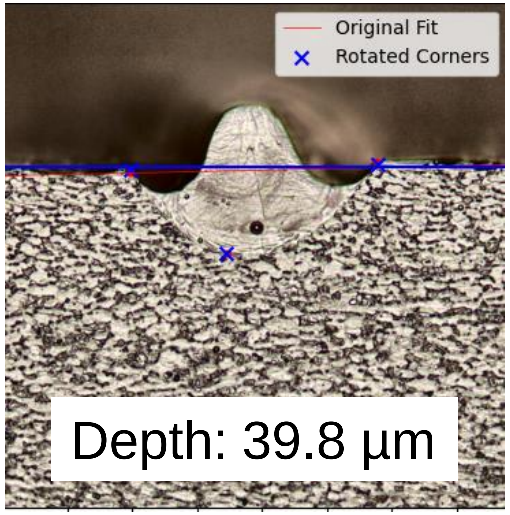
Physical samples and image acquisition

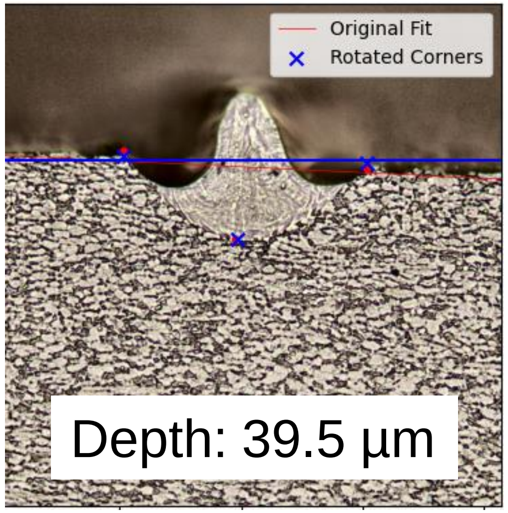
- Dr. Albert To and Seth Strayer (University of Pittsburgh)
- J. Andrew Newman and Harold Claytor (NASA Langley Research Center)

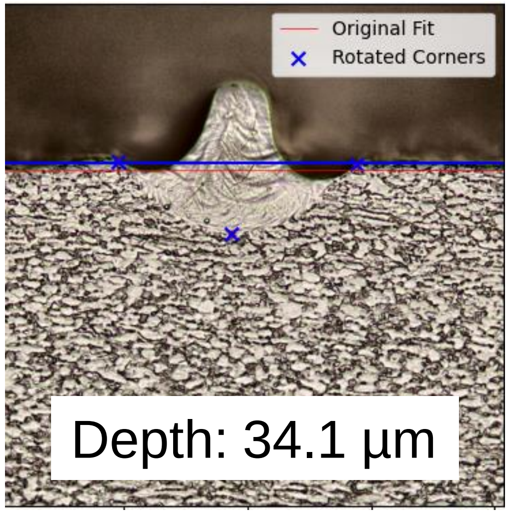
Trends in Melt Pool Depth: Example with Pad 1, Scan 6

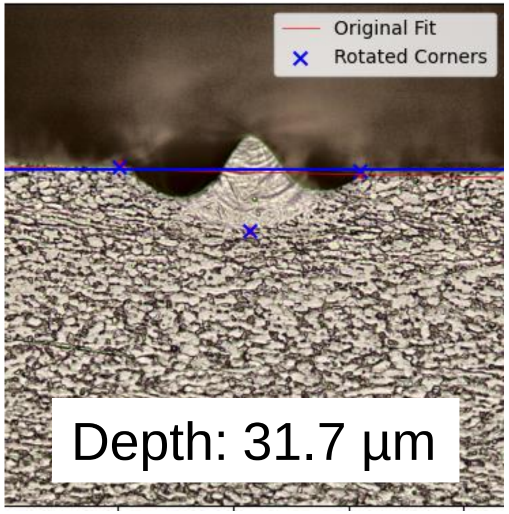
Slice 1


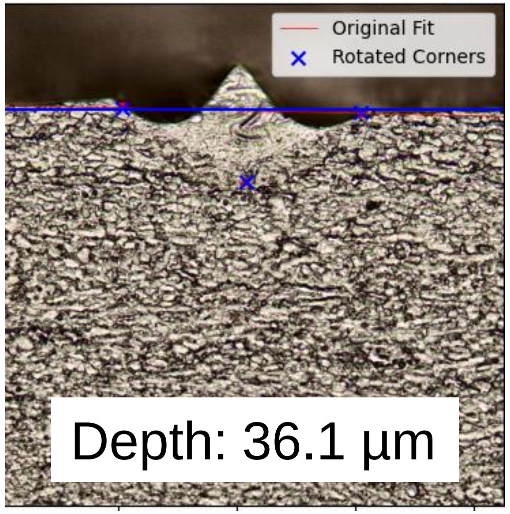
Slice 2


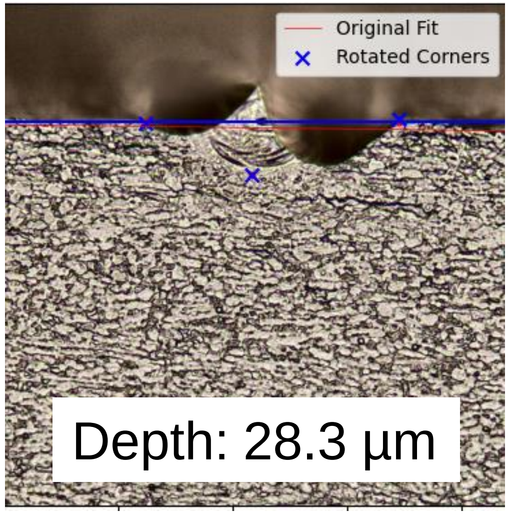
Slice 3


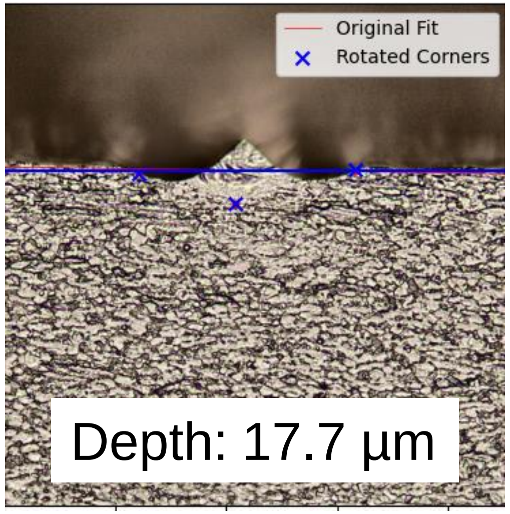
Slice 4


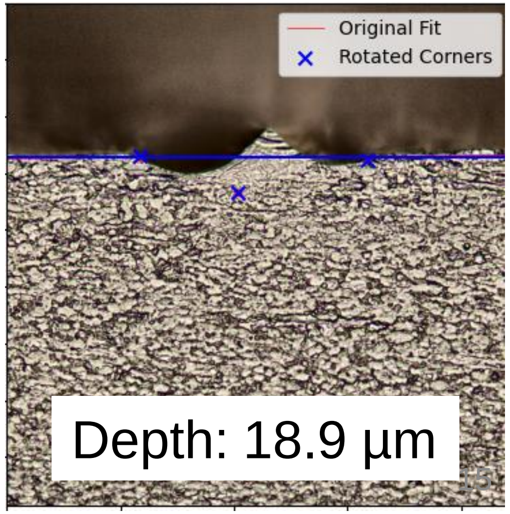
Slice 5


Slice 6


Slice 7


Slice 8


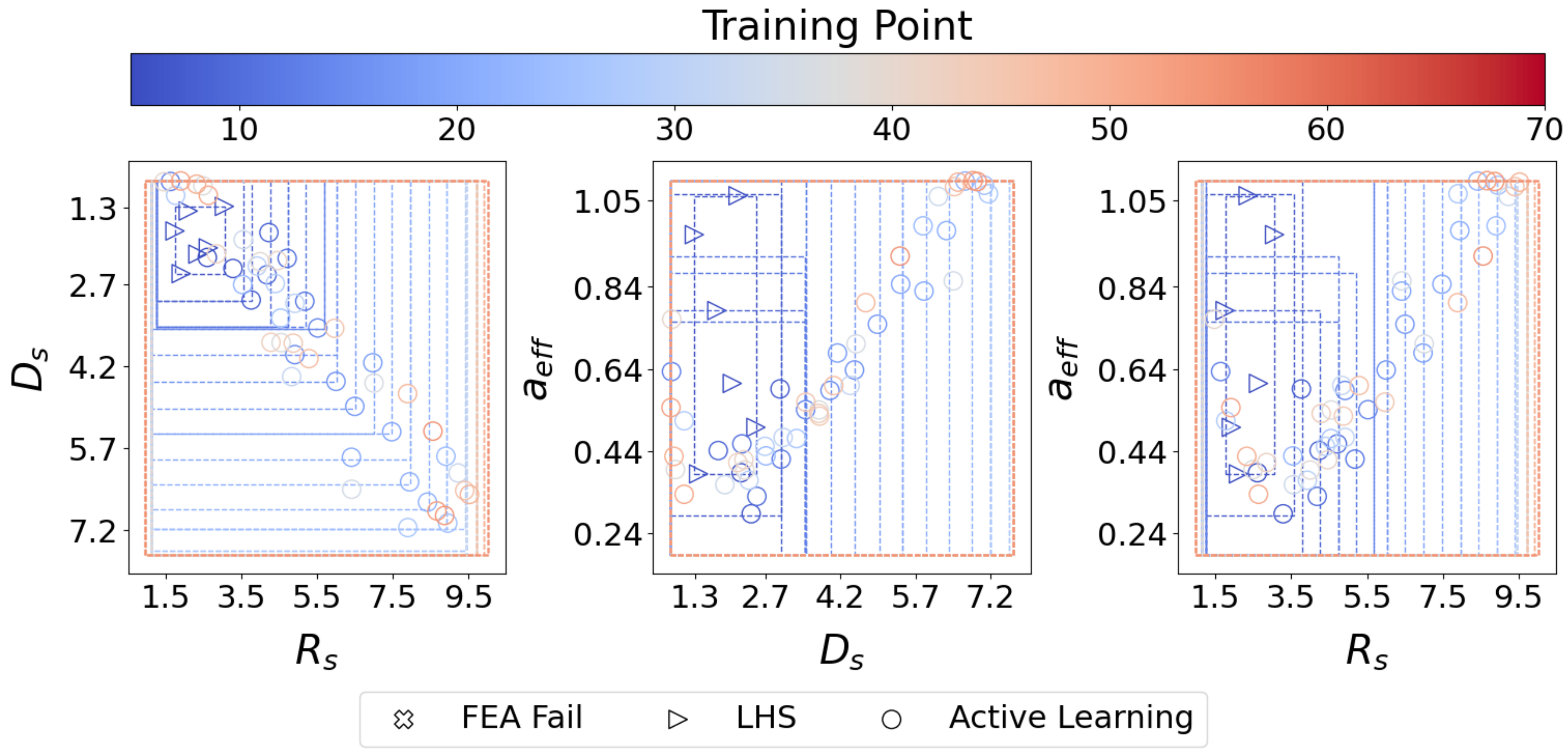
Slice 9


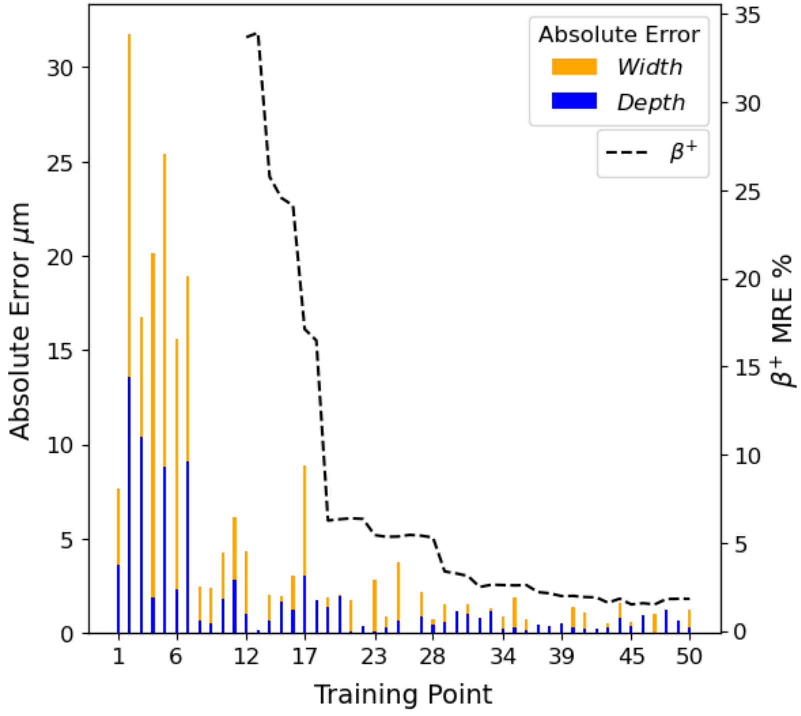
Slice 10


FE Model Calibration Paradigm Training (Scan 5)

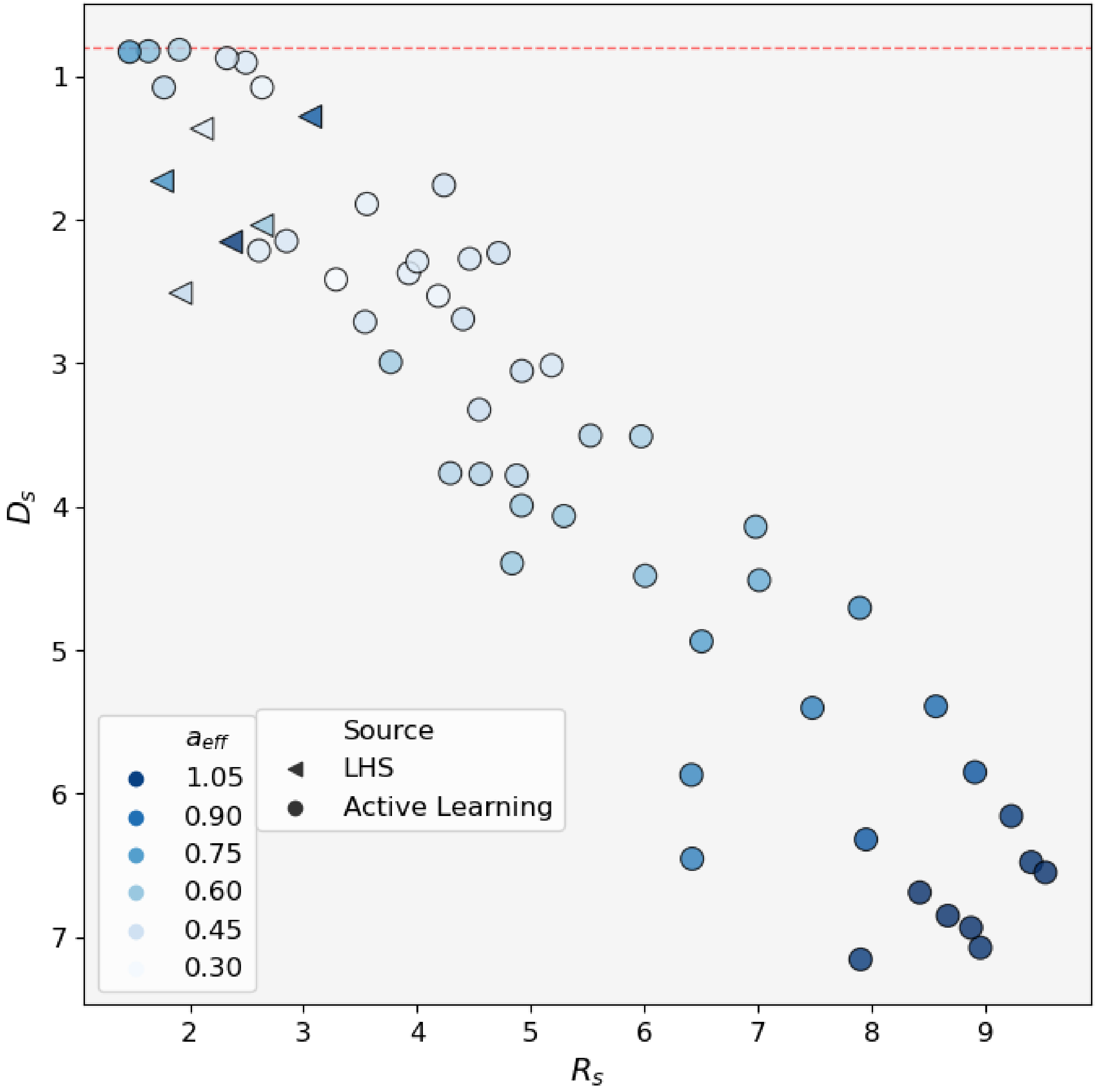
Calibration training process:

- Adaptive prior bounds automatically adjust (below) to focus active learning
  - Gaussian Process Regression (surrogate model) extrapolates to 0
  - Accelerates convergence and reduces fails
- Convergence determined by stability criterion for upper Bollinger Band® of percent mean relative error (β^+ MRE %) of iterative training points (right)





Backup: Scan 5 Training Point Distribution



Backup: Scan 5 Surrogate Contour Plot